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Optimizing a neutron-beam focusing device for the direct geometry time-of-flight spectrometer TOFTOF at the FRM II reactor source

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A B S T R A C T

A dedicated beam-focusing device has been designed for the direct geometry thermal-cold neutron time-of-flight spectrometer TOFTOF at the neutron facility FRM II (Garching, Germany). The prototype, based on the *compressed Archimedes' mirror* concept, benefits from the adaptive-optics technology (adjustable supermirror curvature) and the compact size (only 0.5 m long). We have simulated the neutron transport across the entire guide system. We present a detailed computer characterization of the existing device, along with the study of the factors mostly influencing the future improvement. We have optimized the simulated prototype as a function of the neutron wavelength, accounting also for all relevant features of a real instrument like the non-reflecting side edges. The results confirm the "chromatic" displacement of the focal point (flux density maximum) at fixed supermirror curvature, and the ability of a variable curvature to keep the focal point at the sample position. Our simulations are in excellent agreement with theoretical predictions and the experimentally measured beam profile. With respect to the possibility of a further upgrade, we find that supermirror coatings with *m*-values higher than 3.5 would have only marginal influence on the optimal behaviour, whereas comparable spectrometers could take advantage of longer focusing segments, with particular impact for the thermal region of the neutron spectrum.

1. Introduction

Neutron optics experienced a considerable development over the last decade, thanks to the introduction of non-linearly tapered guide components and the high quality achieved for the commercial supermirror coatings [1]. However, fixed-curvature ballistic guide systems are affected by chromatic aberration. Not only the finite-size divergent source causes a discrepancy between the geometrical focus and the optical focal point (flux density maximum), but the latter also moves as a function of the wavelength. A rationale for this is provided in Ref. [2-3]. In the case of chopper spectroscopy, only a tuneable guide geometry can compensate this effect. This is realized with the so-called adaptive optics technology, commonly employed e.g. for reflective telescopes or X-ray optics, where the presence of mechanical actuators allows changing the supermirror curvature. In the case of neutrons, the wavelength-dependent supermirror curvature accounts for the gravitational corrections too.

In this paper, we study the focalization of a neutron beam achievable with a compact flexible device like the one developed for the neutron spectrometer TOFTOF at the FRM II reactor source (Garching, D). The design is based on the *compressed Archimedes' mirror* concept and exploits the focusing properties of specific parabolic segments for finite-size sources [2]. All technical and mechanical details about the construction of the prototype are contained in Ref. [3], including the performance within real experiments. Here we just mention that, upon replacing less than 5% of the instrument guide length, a wavelength-dependent intensity gain factor between 1.3 and 2 and a gain in signal-to-background ratio between 2 and 14 could be achieved. A central objective in this work has been to provide a careful comparison between simulation results and experimental data, thus assessing the ability of the simulations to reproduce the experimental features. This is a fundamental aspect by the improvement of an already existing instrument, always requiring a preliminary quantitative estimation of feasibility and utility of a possible upgrade. Hence, we treat the device as an existing successful guide component and keep the accent of the discussion on the computational counterpart. The reproducible agreement between neutron Monte-Carlo ray-tracing simulations and neutron imaging measurement confirms the reliability of the simulations over the entire optimization process. This detailed comparison between theory

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and measurements serves as model study for the design of similar and related instrumentation as well as the further improvement of the existing ones. We report that an upgrade of the focusing device with higher m-value supermirrors would do little to enhance the performance of the adaptive focusing device, whereas another, longer, focusing device could be constructed to provide more neutron flux on a small area.

2. Simulation method and instrument model

The main method in this work has been Monte Carlo ray-tracing simulations of the neutron optics, comparing the results with neutron diagnostic measurements on the actual TOFTOF spectrometer. All simulations in this work were carried out with the McStas Monte Carlo ray-tracing package, version 1.12c [4]. In our modelling, we have used only standard McStas components.

2.1. Simulation set-up

The simulated TOFTOF instrument contained a close model of the TOFTOF guide-chopper system [5], where only the last 0.5 m segment has been replaced with the new focusing element. The neutron source reproduces the flux distribution of the FRM II seen at TOFTOF, and has been employed for all previous optimization of the instrument [6,7].

The original neutron guide system uses commercial optics. It consists of a cascade of linearly tapered focusing elements extending across the chopper system. The chopper slits follow the decrease of the guide cross-section, and the supermirror coating increases accordingly from $m=2$ (before the first chopper) up to $m=3.5$ in front of the sample. The last segment of the neutron guide, 495 mm long, is contained in the so-called "exchange guide". The latter consists of a 502 mm-long box, placed after the last chopper, hosting two vertical stages for different guide options: a straight linear collimator and a linearly tapered focusing guide (namely, a "trumpet"). A stepping motor allows the vertical translation, thus switching between the two options (see Fig. 1).

The focusing prototype replaces the former straight linear collimator. It has been realized completely at the FRM II, including the supermirrors with coating $m=3.5$ [8]. We outline the main geometrical aspects relevant for the simulations. The prototype consists of four independent walls, each one connected to a piezomotor. The device has everywhere a rectangular cross-section, fixed at the entrance and variable at the exit: it narrows towards the sample position according to a third-order polynomial deformation impressed by the piezomotors. The exact deformation is described in Ref. [3]. However, for the purpose of this discussion, it is relevant only that the short segment of interest can be well approximated by a parabola, thus granting the applicability of

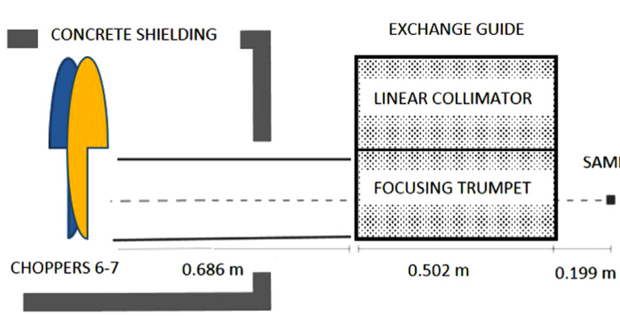

Fig. 1. A sketch of the traditional TOFTOF neutron guide system between the last chopper pair and the sample. From the left to the right: After passing the monochromatizing double choppers, the neutrons reach a fixed linearly tapered component, extending across the shielding wall, and then enter the exchange guide.

the *compressed Archimedes' mirror* concept [2]. The profile of each wall has been cut according to the equation of the maximal deformation, in a way that at the maximal simultaneous curvature, all mirrors match exactly without colliding. For the same reason, at any intermediate curvature, small side gaps open along the guide edges. From a practical as well as computational point of view, this is the equivalent of the much more common case of non-reflecting side edges, as machined during the supermirror substrate processing. We progressively refined the layout of the optical components, from the ideal mathematical description towards (a) a set of linearly tapered pieces and (b) a "real" tuneable focusing device, whose mirrors can be bent but not stretched, thus introducing gaps along the four longitudinal side edges. Both options (a) and (b) approximate the polynomial deformation with a spline. Several Figures-of-Merits (FoM) have been taken into consideration. Among others, we mention a self-implemented monitor "Brilliance/FWHM", particularly useful for detection of the chromatic aberration. This is based on a conventional McStas PSD intensity monitor, the FWHM being the full width at half maximum of the simulated beam spot. Upon weighting the inverse of the FWHM by the monochromatic brilliance, we simultaneously minimize the FWHM and maximize the brilliance of the beam. During these optimizations, we realized that most of such FoMs were leading to equivalent results, as part of the optimization was already done with the initial conceptual design. Therefore, we decided to rely on the beam intensity in a $10 \times 10\ \mathrm{mm}^2$ area at the sample position. We did not take into account a penalty for those neutrons missing the sample so badly that they would reach the bulky sample environment. The simulations sampled the whole thermal-cold range, at the reference wavelengths of 1.5, 3, 6, 9 and 12 Å.

2.2. Chromatic aberration

The effects of chromatic aberration can be considered from two different viewpoints. On one side, at fixed curvature the focal point moves as a function of the incoming wavelength. The displacement is of the order of several centimetres for the typical TOFTOF wavelength range [3,8] and, in the limiting case, could lead to the focus being closest to the sample environment. On the other side, if one wishes to maximize the intensity gain over the smallest possible area at a fixed position (say the sample), it is found that the optimal curvature of the guide varies with the wavelength. The first approach represented the guideline for the conceptual design of the focusing device [3,8], whereas the second approach defines the detailed optimization process carried out with the present study.

The first detailed analysis of the chromatic aberration with direct geometry time-of-flight spectroscopy over a broad-bandwidth thermal-cold range can be found in Ref. [3]. By means of a unique compact device, we managed to improve the performance of the instrument at each wavelength, without affecting the properties of the chopper system and preserving the standard TOFTOF configuration as an option. Previously, similar problems had been debated only for triple-axis spectroscopy [9,10] and neutron reflectometry [11,12], where it is much easier to separate the monochromatizing mechanism from the properties of the neutron guide. The only successful attempt for chopper spectroscopy had been the design of a fixed-geometry, multi-channel focusing segment optimized for a cold wavelength of interest [13].

We have performed an iterative crosscheck between simulated and experimental beam intensities. First, we applied this procedure to the wavelength-resolved optimization of the curvature of the existing focusing prototype, as these results could be compared with the experimental measures. Once we got the control on the role of each parameter, we moved a step further towards a deeper conceptual revision of the spectrometer.

2.3. Measuring the neutron beam at TOFTOF

The results of McStas simulations were compared with neutron images taken at TOFTOF with a neutron sensitive CCD camera built at the FRM II: a so-called "DEL-Cam". We optimized the curvature at several wavelengths in the thermal-cold range 1.5–12 Å. We bent the supermirrors according to curvatures indicated by the McStas optimization and measured the beam profiles at the real instrument. We note that the same curvature values could be determined also experimentally, independently from these simulations.

When not differently indicated, the comparison between McStas and neutron imaging was carried out as follows. The vertical intensity profiles were obtained by integrating the intensity of a vertical strip, centred at the sample position, over a horizontal width of 1 cm. The horizontal profiles were similarly obtained by vertical integrating over a horizontal 1 cm tall strip. Experimental data were normalized to the acquisition time and the flux. The simulations were normalized to the number of neutron rays, as is standard in McStas.

3. Simulation results

Here, we present the results of the McStas simulations and compare them with neutron imaging data taken at TOFTOF. We report the results from the existing focusing device and its future improvement in two dedicated sections, according to the two options indicated in Fig. 2. The first section is mostly centred on the performance in the cold wavelength range. For simplicity, and without loss of generality, the results are discussed only for 6 Å neutrons. The second section is devoted to the future perspective for thermal neutrons. Here, the results are discussed with respect to the entire wavelength range of TOFTOF.

3.1. The present focusing device

We started with the calibration of the entire comparison procedure, using the set-up of the traditional TOFTOF configuration with the focusing trumpet. The intensity ratios between the

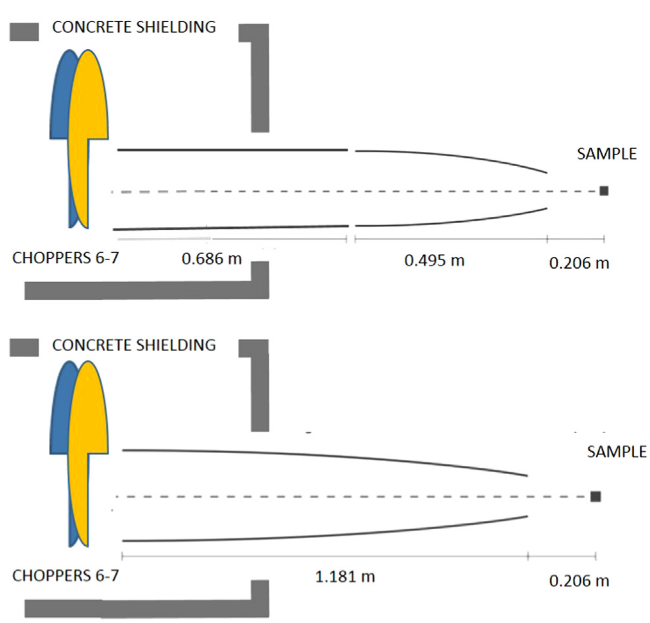

Fig. 2. Schematic view of the two different focusing configurations we simulated: (top) the current prototype (bottom) a much longer device, starting immediately after the last chopper pair.

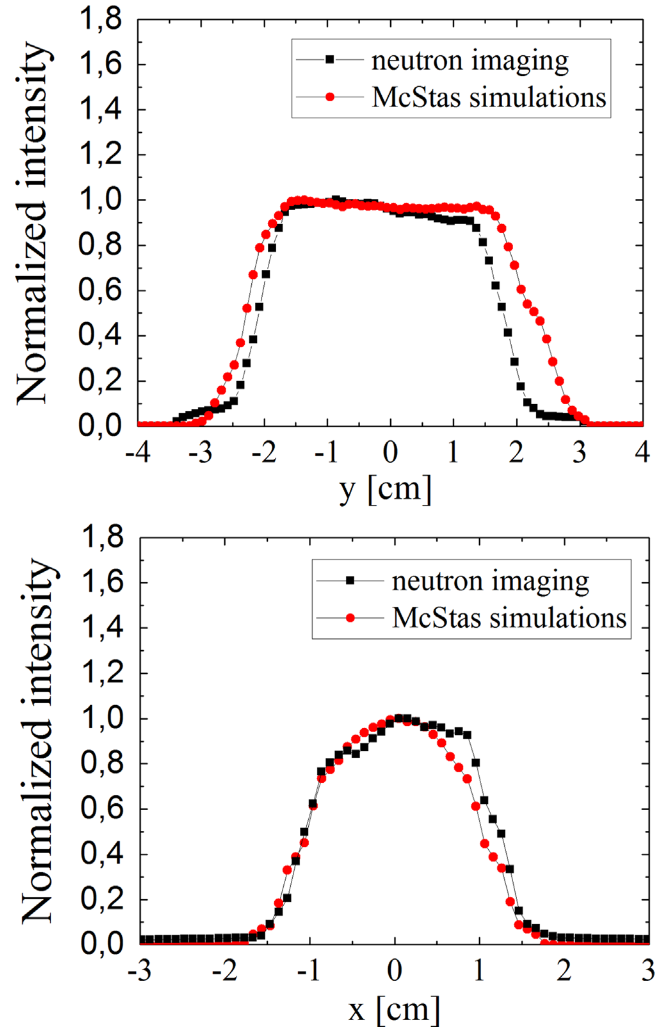

Fig. 3. Validity and consistency check between McStas simulations (squares) and neutron imaging at the TOFTOF (circles). The top panel shows the vertical intensity profile, while the bottom panel shows the horizontal profile. Measurements were taken with the linear trumpet using a neutron wavelength of 6 Å.

McStas data and the neutron imaging data provided the scale factors for the wavelengths of interest. They mostly account for the detection efficiency of the DEL-Cam, and have been imposed to the comparison of the results obtained for the focusing device.

The validity check of the calibration at 6 Å is shown in Fig. 3. The slightly narrower experimental profile in the vertical direction is due to the presence of slits, mounted at the exit of the guide in the real instrument. These avoid the extreme illumination of the sample environment at long wavelengths, where the beam has the highest divergence. The employment of the non-linear focusing geometry will eliminate the need for these slits.

The comparison with the focusing device is reported in Fig. 4 at 6 Å. In the experimental data, we observe a slightly less pronounced intensity maximum along the vertical direction and redistributed scattering intensity. This is a cumulative result of some minor local misalignments in the rest of the guide system, as typical of real chopper spectrometers in routine operation. Within the normalization, the discrepancy between simulated and measured data is only few percent of the integrated intensity. Data at other wavelengths are presented in a thorough description in Ref. [3].

Here we discuss the excellent qualitative and quantitative agreement between simulation and experiment, facilitated by the implementation in McStas of a realistic focusing device

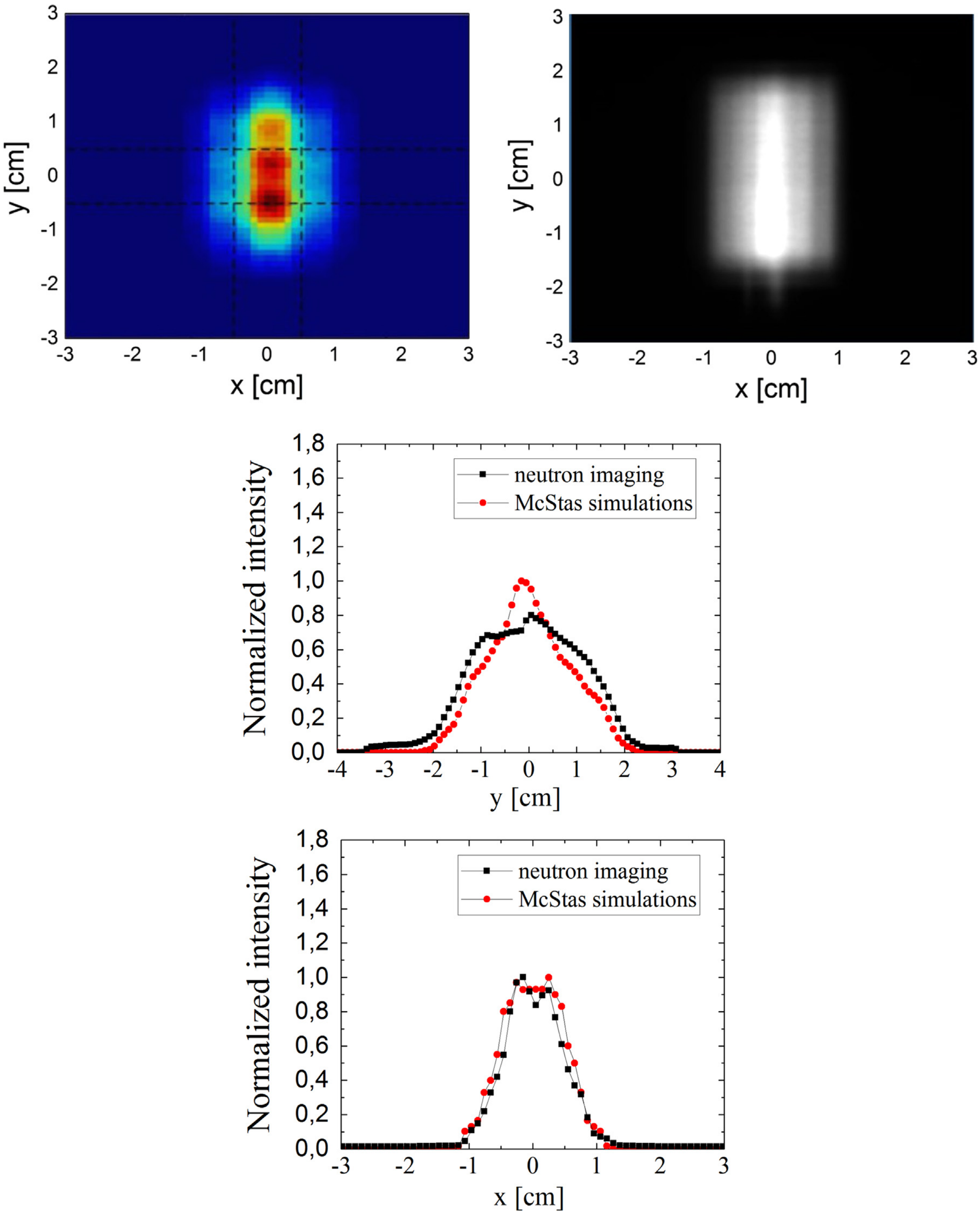

Fig. 4. Comparison between McStas simulations and neutron imaging with the focusing prototype at 6 Å. Simulations performed with choppers running at the same experimental settings and at the optimal curvature. From top to bottom: the simulated PSD intensity-monitor; imaging with the DEL-Cam; vertical intensity distribution; and horizontal intensity distribution.

component with open side edges. McStas standard components either contain gravity corrections and realistic side edges or support the definition of specific guide curvatures. Then we approximated the supermirror curvature with a spline, and implemented a cascade of linearly tapered components (2 cm long) with non-reflecting chamfered side edges. First, according to the McStas manual, a series of short components is the best way of simulating a realistic guide. Second, this allowed using only the standard *guide gravity* component. The size of the side gaps (chamfered edges, in the simulations) depends on the guide curvature, i.e. on the neutron wavelength. Moreover, at fixed curvature the size varies along the device length, as an effect of the non-linearity of the curvature. Only at the maximal curvature the device is perfectly closed, with no side gaps and therefore no chamfers. We used this information for constraining the size of the non-reflecting edges at any intermediate curvature. At each wavelength, we calculated the deviation of the corresponding guide cross-section from the maximal curvature, we approximated the deviation function at the same spline points used for the supermirror curvature, and assigned the values to the vertical/

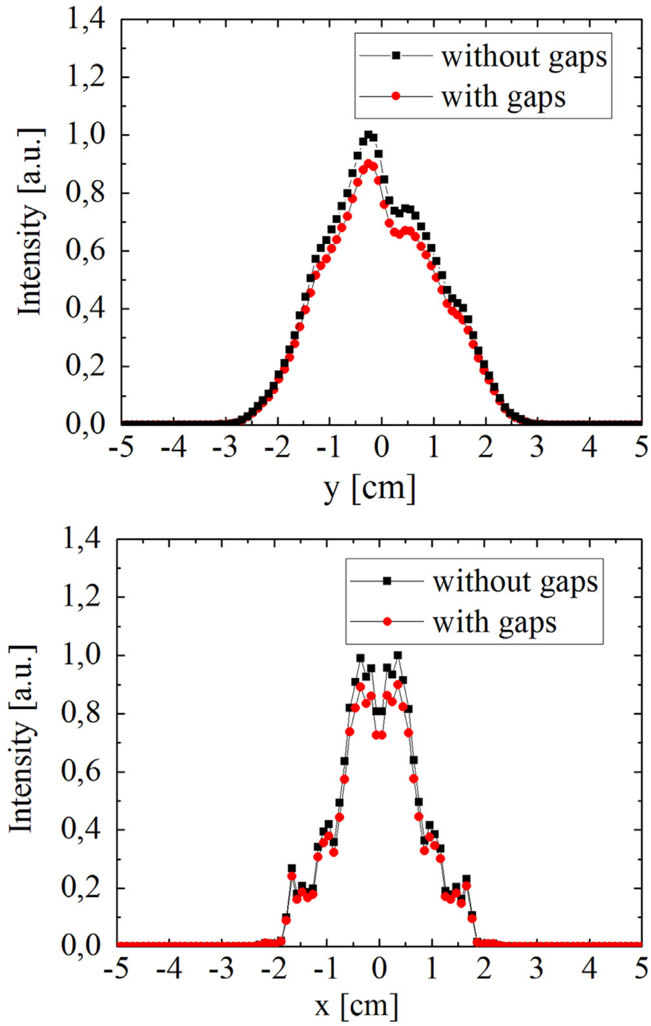

Fig. 5. The effect of introducing side gaps in the focusing device, simulated for 12 Å neutrons: (top) vertical intensity distribution and (bottom) horizontal intensity distribution.

horizontal chamfers of the related linearly tapered guide segment. The results of these simulations are found in Fig. 5. The role played by these corrections scales with the divergence distribution, and therefore the wavelength, thus reaching its maximum at 12 Å. At that limit, the effect of the non-reflecting corners is at most a 10% of the absolute intensity, becoming negligible below 6 Å. Moreover, the general shape of the reflectivity curves does not change when the non-reflecting corners are included.

3.2. Designing the new focusing device

With the present focusing prototype short wavelengths already benefit from an improved signal-to-background ratio. However, as discussed in [3], at $\lambda < 4$ Å this is mostly due to a dramatic reduction of the background contribution, achieved by reducing the illumination of the sample environment. The main driving force for a further development of focusing devices for TOFTOF has been the need to increase the neutron flux also at $\lambda < 4$ Å without affecting the performance at the other wavelengths. $\lambda < 4$ Å are routinely used for inelastic neutron scattering (INS), where typical signal intensities are quite low compared to the elastic line. For good data analysis in INS, a good neutron statistics is required. This is available e.g. by much higher beam intensities, which non-linearly tapered focusing guide systems can provide. Hence, our ultimate goal has been a gain in signal intensity and signal-to-background ratio comparable to the one already achieved for quasi-elastic scattering (QENS) for $\lambda > 4$ Å [3].

The enhancement of the neutron flux is obtained at the cost of a higher divergence of the beam though, and the right compromise must be found on each specific instrument. Based on the current TOFTOF detector bank and at the typical scientific applications and resolution requirements, we defined the “useful neutrons” to be those with divergence $\pm 1.5°$, both vertically and horizontally. According to this criterion, which we will discuss in more detail in the following, we optimized the configuration of the existing device and investigated the influence of the different factors: the shape, the supermirror coating and the guide length.

3.3. Shape

We considered the performance of standard McStas non-linearly tapered components, i.e. ellipse and parabola, starting from their best approximation of the existing focusing device. The results confirmed what found in [3,8]: the intensity gains are comparable, but the parabolic guide provides a much more homogeneous flux distribution at the sample position.

3.4. Supermirror coating

As far as the coating is concerned, we performed simulations with varying m-quality up to the limit of the large-scale commercial feasibility, i.e. $m=6$. In all simulations, we used the reflectivity model

$$R(q) = \begin{cases} 1; q < q_{c,\mathrm{Ni}} \\ 1-\alpha(q-q_{c,\mathrm{Ni}}); \quad q_{c,\mathrm{Ni}} < q < mq_{c,\mathrm{Ni}} \\ 0; q > mq_{c,\mathrm{Ni}}, \end{cases} \tag{1}$$

where all the reflectivity curves $R(q)$ overlap for $q < mq_{c,\mathrm{Ni}}$. We have used the default value $\alpha=4.38$ for all guides. This expression favours high m-values, since the real reflectivity values for medium q-values is slightly lower for high m-values than for medium m-values [14]. However, as we shall see, this approximation does not seem to visibly bias the optimizations towards the high-m direction. Fig. 6 shows the performance at four significant wavelengths.

At each wavelength, we compared the intensity of low-divergence neutrons with that of all divergences, and presented them as a function of m-value. Our analysis considered the interplay between supermirror coating, neutron divergence, energy resolution and background contribution. This can be understood as follows. The secondary spectrometer of TOFTOF works in direct geometry. Moreover, the detector bank has no position sensitive detectors, but 40 cm-long ^{3}He tubes, mounted at 4 vertical orders. The tubes cover the surface of the scattering sphere, 4 m radius, centred at the sample position, and the out-of-plane alignment follows the intersections with the Debye–Scherrer cones. The original guide-chopper system had been optimized accordingly. In the case of TOFTOF only neutron divergences up to $\pm 1.5°$ preserve a good resolution ellipsoid for INS, whereas the higher divergences would destroy parts of the experimental information. Moreover, in the case of a finite-size source, higher supermirror coatings allow higher beam focalization but increase also the transfer efficiency for those neutrons responsible for the background. This second aspect is more relevant for cold neutrons, as we will now see upon comparing the results at the different wavelengths.

In the thermal range, 1.5 Å, we observe that the gain is achieved only by “useful neutrons”, as wished. However, upon increasing the coating from $m=3$ to $m=6$, an increase of intensity of only 5% is achieved. This small gain is of questionable scientific impact, and given the increased construction price, this upgrade would be unjustified, when only this wavelength was considered.

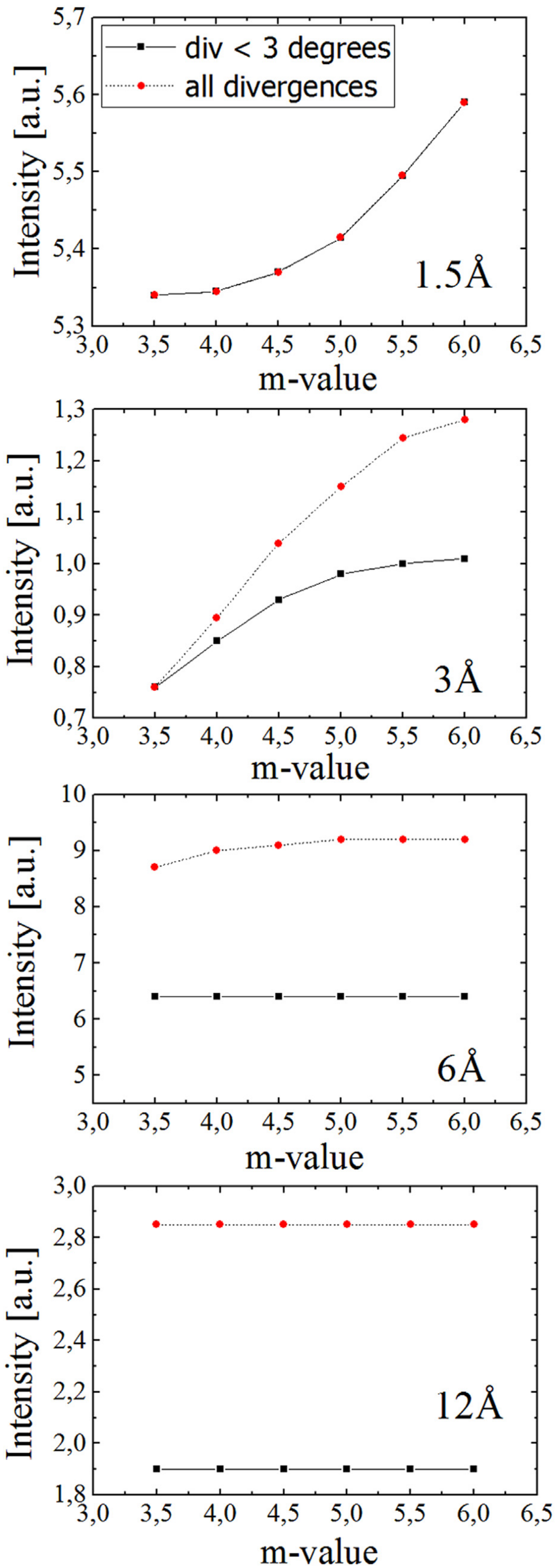

Fig. 6. Effect of the supermirror coating on the beam intensity, presented as a function of neutron wavelength. McStas simulations were performed with the optimal curvature of the current prototype. Black, straight lines represent the intensity of neutrons below the divergence limit, while dotted, red lines represent the intensity of all neutrons. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this paper.)

In the cold range, 6 Å and 12 Å, the coating has really no influence, as the reflectivity of the focusing device is not at all the limiting factor in the beamline optics.

The simulations for 3 Å neutrons show a completely different picture with an increase of useful neutrons on going to higher mirror quality, and a much higher increase of useless neutrons. This validates the correctness of the former conceptual design of the current prototype. The mirror quality $m=3.5$ is seen to be the value which provides an intensity gain with respect to the linear trumpet, while still filtering exactly all neutrons with divergences higher than $\pm 1.5°$. We conclude from this study that there is no need to replace the present $m=3.5$ mirrors with more expensive, high coating supermirrors.

3.5. Length

Finally, we considered the possibility of a much deeper revision of the instrument, while preserving the properties of the existing chopper system. Assuming to accept a permanent upgrade of TOFTOF, without the possibility of switching between two options, a much longer guide piece could be installed. This could extend from the last chopper up to the exit of the exchange guide, for a total length of about 1.2 m. We considered a parabolic shape approximating the current prototype, we kept the coating fixed at m=3.5 and increased the length from 0.5 m up to 1.2 m. Fig. 7 shows the performance in the thermal region. The factor 2.4 in the total length would result in an average intensity increase of +70%, without loss of focalization in any direction. Such a result confirms the analogies between refractive visible-light optics, reflective neutron optics, and scattering-based detection methods underlined in [3] when discussing the focusing efficiency of the device. Indeed, at a given guide length, we observed that the longer the neutron wavelength, the slower the probe, the most efficient the interaction with the (focusing) medium. Thanks to these detailed McStas simulations, we coherently conclude that the best way for increasing the optical depth at the shorter wavelengths is an increase of the optical thickness (i.e. the guide length) of the focusing neutron segment.

4. Conclusion

By means of iterative comparison between McStas and neutron imaging at TOFTOF, we have developed a realistic model of the current focusing prototype. We have achieved an excellent, qualitative and quantitative agreement between simulated and measured performance of the whole spectrometer. This confirms the reliability of the McStas calculations.

The different simulation sessions have allowed us to investigate the specific role of the real features of chopper spectroscopy and adaptive optics on the overall neutron transfer. We find that the side gaps opening at the intermediate curvature of the supermirrors have minor influence on the intensity loss, which is at most a 10% and can be neglected for wavelengths shorter than 6 Å. The investigation of a deeper upgrade of TOFTOF has provided quite promising results. It turns out that an increase of the supermirror quality will not affect the neutron flux, whereas the latter is quite sensitive to the length of the parabolic segment. This fact is particularly relevant for TOFTOF, due to its technical feasibility: it would allow almost doubling the flux in the thermal region, without changing anything in the rest of the wavelength range. These results will be taken into account for the future improvement of TOFTOF, and will serve as guidelines for the design of similar spectrometers.

Our findings are in fair agreement with visible-optics equivalents as well as recent results of guide simulations, which have

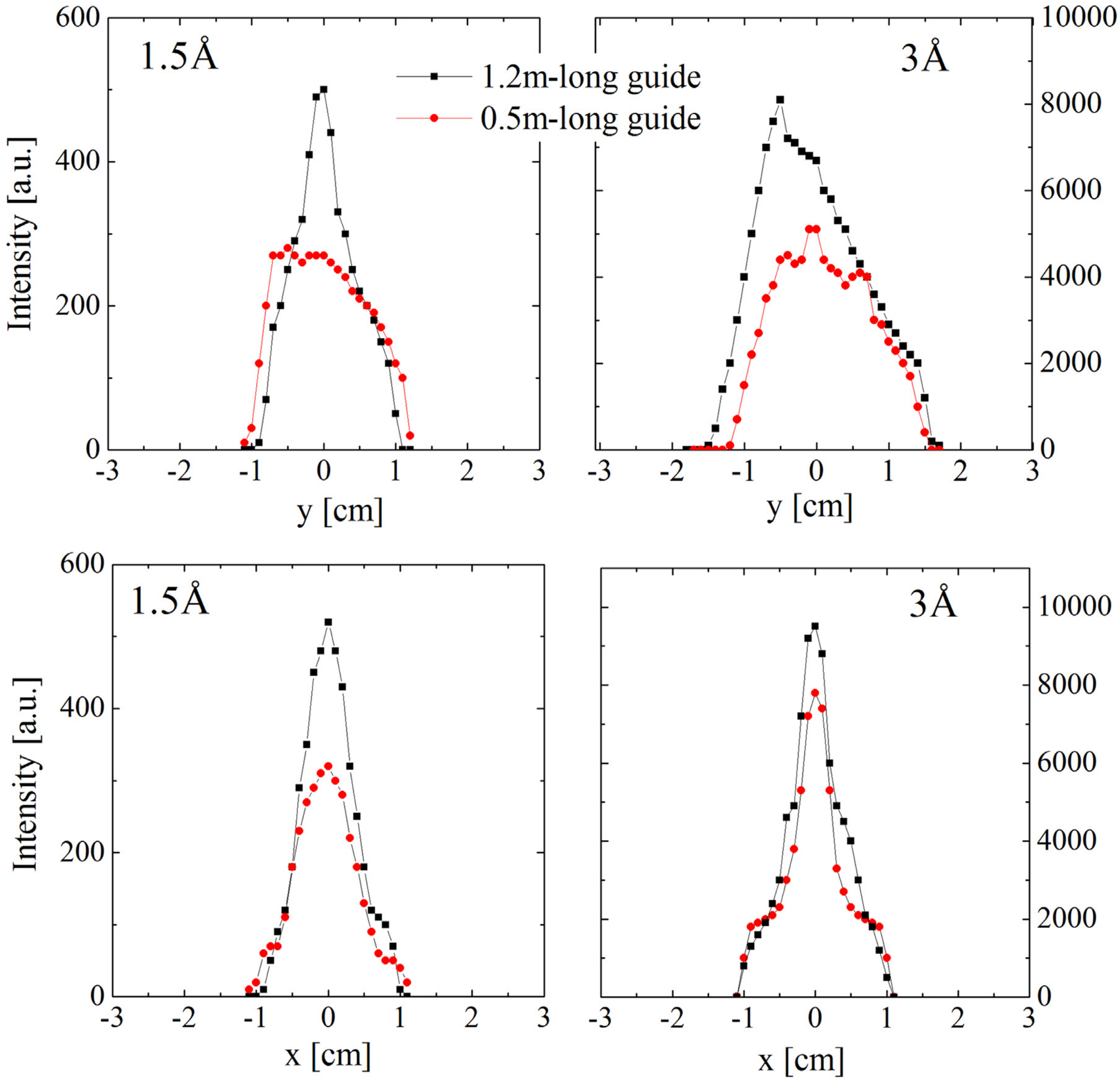

Fig. 7. Effect of the length of the guide for the transport of short wavelengths. The data show McStas simulations with parabolic devices of 0.5 m and 1.2 m length. Simulations were performed at neutron wavelengths of 1.5 Å (left) and at 3 Å (right). Top panels show the vertical intensity distributions, while bottom panels show the horizontal intensity distributions.

proved the intrinsic higher performance of longer ballistic guides of any geometry compared to shorter guides [15,16].

Acknowledgements

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